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Efficient real-space approach to TDDFT for the dielectric response of periodic systems

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Time-dependent density functional theory has been used to calculate the static and frequency-dependent dielectric function of non-metallic crystals. We show that a real-space description becomes feasible by using a lattice-periodic (microscopic) scalar potential in combination with a uniform (macroscopic) electric field. The induced density and microscopic potential can be obtained self-consistently for fixed macroscopic field by using linear response theory, in which Coulomb interactions and exchange-correlation effects are included. The induced polarisation (and hence the dielectric function) can then be obtained from the induced current.

We obtained the dielectric function for a wide range of materials within the adiabatic local density approximation in good agreement with experiment. The accurate results for the low-frequency range show that no adjustment of the LDA band gap seems to be necessary. Spectral features of the dielectric function appear in the calculations with the correct strength and shape, however, at more or less uniformly shifted energies.

References

- 'Efficient Real-Space Approach to Time-Dependent Density Functional Theoryfor the Dielectric Response of Non-Metallic Crystals', F. Kootstra, P. L. de Boeij and J. G. Snijders.
  submitted to J. Chem. Phys. 7 okt. 1999

- 'Application of Time-Dependent Density Functional Theory to the Dielectric Function of various Non-Metallic Crystals', F. Kootstra, P. L. de Boeij and J. G. Snijders.
  submitted to Phys. Rev. B. 14 dec. 1999